

# Recent Progress in the Theory of the Crystalline Undulator

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## Abstract

If an ultrarelativistic charged particle channels inside a single crystal with periodically bent crystallographic planes, it emits hard electromagnetic radiation of the undulator type. Due to similarity of its physical principles to the ordinary (magnetic) undulator, such a device is termed as the crystalline undulator. Recent development of a new Monte Carlo code ChaS made possible a detailed simulation of particle channeling and radiation emission in periodically bent crystals. According to recent findings, energy of the electron beam below 1 GeV is sufficient to observe the undulator effect in a periodically bent crystal. Even more exciting results were obtained for a crystalline undulator whose bending period is shorter than the period of the channeling oscillations and the bending amplitude is smaller than the width of the planar channel. Such a crystalline undulator is far superior to what was proposed previously. It allows for a large effective number of undulator periods. Therefore, it is predicted to emit intense undulator radiation in the forward direction. A narrow undulator peak is seen for both positron and electron beams. Using positrons is, however, more desirable because in this case the intensity of the undulator radiation is higher while the background is lower.

**Keywords:** channeling, radiation by moving charges, crystalline undulator, channeling radiation, electron and positron beams, synchrotron radiation sources, Monte Carlo method, strained layer superlattice

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The idea of the crystalline undulator (CU) was proposed more than three decades ago [1, 2, 3, 4]. It was suggested to use a periodically bent crystal to generate hard electromagnetic radiation of undulator type. Ultrarelativistic electrons or positrons were supposed to channel through such a crystal following the sinusoidal shape of the bent crystallographic planes. Due to nearly harmonic transverse oscillations of the particles, the electromagnetic waves emitted in the forward direction were expected to have a narrow spectral distribution, similarly to an ordinary (magnetic) undulator [5, 6, 7].

The extremely strong electromagnetic fields inside the crystal can steer the beam particles much more effectively than it would be possible even with the best superconductive magnets. Therefore, the period of the crystalline undulator can be made orders of magnitude smaller than that of the magnetic undulator. Hence, the crystalline undulator is potentially capable of generating hard X rays and gamma rays.

There is, however, a price to pay for taking advantage of the crystalline field. In contrast to the ordinary undulator, the particles move in a dense medium instead of vacuum. They experience random collisions with crystal constituents and, therefore, they emit bremsstrahlung which may constitute a substantial background. Coherent effects contaminate the spectrum even stronger. In addition to undulator oscillations, the particle has to perform channeling oscillations around the minimum of the planar potential (similarly to its motion in a straight crystal). As a result, channeling radiation is present in the spectrum of

the crystalline undulator in addition to undulator radiation and bremsstrahlung.

Channeling radiation has a lot in common with undulator radiation [8]. Therefore, even a straight crystal can be used to build a source of hard photons. However, this approach has a disadvantage. Because the shape of the transverse potential is not parabolic, the transverse motion of the particles is not harmonic. As a result, the spectrum of the channeling radiation is broader than that of the undulator radiation, especially in the case of negatively charged projectiles.<sup>1</sup>

An interesting phenomenon of narrowing the planar channeling radiation peak has been observed for positrons [13, 14]. The reason is a partial compensation of the potential inharmonicity by deviations from the dipole approximation in the radiation emission [15]. This takes, however, place only at a certain 'magic' beam energy. This means that the position of the narrow peak is fixed for every crystal channel, i.e. the radiation frequency can be varied only within a very limited interval.

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<sup>1</sup> Another difference between channeling radiation and undulator radiation is that the latter one can be coherent if the particle beam is modulated (bunched) in the longitudinal direction with the period equal to the wavelength of the undulator peak. In this case the different particles radiate electromagnetic waves with nearly the same phase. Therefore, the intensity of the radiation becomes proportional to the number of particles squared (in contrast to a linear proportionality for an unmodulated beam). This way of producing coherent radiation is utilized in free electron lasers [9] (see e.g. [10] for a modern review). Similar effect should be observed in a crystalline undulator if it is fed by a bunched particle beam [11, 12]. In contrast, channeling radiation will not become coherent even in the case of a modulated beam because the phases of the channeling oscillations are arbitrary and random.

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The CU approach does not have such restrictions. The undulator radiation peak can be shifted within a wide range of values by varying the beam energy and the bending period. But one has to put up with the contamination of the spectrum by channeling radiation unless one finds a way to get rid of it.

The radiation background is not the only challenge faced by the CU. It was realized at the very beginning [4] that the effective length of the crystalline undulator is limited by the attenuation of photons in the crystal medium. This limitation is, however, essential if rather soft photons,  $\hbar\omega \lesssim 100$  keV are to be produced.

A more severe restriction on the effective length of the bent crystal is imposed by the dechanneling phenomenon [16]. The incoherent bremsstrahlung is not the only undesirable effect of random scattering of the projectiles by the crystal constituents. Due to the random collisions, the transverse energy of the channeling particle fluctuates. Positive fluctuations are, however, more likely than negative ones. Therefore, the projectile gains on average the transverse energy. If the latter exceeds the height of the interchannel potential barrier, the particle leaves the channel [17]. Starting from this point, it does not follow the shape of the channel and, consequently, it does not emit undulator radiation. For this reason, the effective number of undulator periods  $N_u$  is limited by the average length  $L_d$  at which the dechanneling takes place:

$$N_u \simeq \frac{L_d}{\lambda_u}, \quad (1)$$

where  $\lambda_u$  is the bending period of the crystalline undulator. The number of undulator periods has to be large,  $N_u \gg 1$ , to ensure a narrow spectral distribution of the undulator radiation. Therefore, the following condition has to be satisfied by the undulator period

$$\lambda_u \ll L_d. \quad (2)$$

In its initial form, the idea of the CU was based on the assumption that the projectile should follow the sinusoidal shape of the bent crystallographic planes and perform, at the same time, channeling oscillations around the central plane of the channel. This implied that the bending period of the undulator had to be much larger than the period of channeling oscillations

$$\lambda_u \gg \lambda_c. \quad (3)$$

In addition, the undulator bending amplitude  $a_u$  has to be much larger than the typical amplitude of channeling oscillations  $a_c$ . This condition can be rewritten in the form [18]

$$a_u \gg d \quad (4)$$

due to the fact that  $a_c \lesssim d/2$ , where  $d$  is the channel width (the distance between the bent crystallographic planes that form the channel). The strong inequality (4) has to be satisfied to ensure a higher intensity of the undulator radiation relative to the channeling radiation.

In the following, the crystalline undulator satisfying conditions (3) and (4) will be referred to as LALP CU (**l**arge **a**mplitude and **l**ong **p**eriod crystalline **u**ndulator). The complete list of

conditions that have to be satisfied by the parameters of LALP CU can be found in [19].<sup>2</sup>

One more condition is relevant to the present discussion. It ensures a stable channeling of the projectile in the periodically bent crystal of LALP CU [2, 4]. Initially, similar condition was obtained for channels with constant curvature [20]. It is convenient to write it down in the form<sup>3</sup>

$$1 > C \equiv \frac{F_{cf}}{U'_{\max}} = 4\pi^2 \frac{a_u E}{\lambda_u^2 U'_{\max}}. \quad (5)$$

Here  $C$  is the centrifugal parameter [19],  $F_{cf}$  is the maximal centrifugal force acting on the projectile in a the periodically bent channel,  $U'_{\max}$  is the maximal force that keeps the particle in the channel and  $E$  is the energy of the projectile.

Conditions (2), (4) and (5) are difficult to satisfy simultaneously. In particular, they cannot be satisfied in the case of electron beam of moderate energy,  $E \lesssim 1$  GeV. For instance, if one sticks with (3), the most favorable conditions for observing undulator radiation from  $E = 855$  MeV electrons in the Si(110) channel are  $\lambda_u \approx 4 \mu\text{m}$  and  $C \approx 0.3$ . This corresponds to  $a_u \approx 0.84 \text{ \AA}$  ( $a_u/d \approx 0.44$ ), i.e. condition (4) is broken. Taking into account that the dechanneling length  $L_d \approx 8.3 \mu\text{m}$  even for the straight Si(110) channel [21],<sup>4</sup> one sees that the strong inequality (2) is not satisfied either. As a result, the undulator peak is rather small and not very sharp while the spectrum is dominated by the channeling radiation (see figure 1).

Still, it is remarkable that the undulator effect is predicted to be detectable even using electron beams of moderate energies. This awakes expectation that a successful proof of principle experiment can be done in the nearest future, for example, at Mainz Microtrone (MAMI).

The LALP CU conditions can be fulfilled for positron beams (see [19] and references therein) and for high energy,  $E > 10$  GeV, electrons [23].

An example of a spectrum of a positron-based LALP CU is shown in figure 2. The undulator peak is narrow and is substantially higher than the channeling radiation maximum. Nevertheless, the total energy of channeling radiation (integrated over the photon energy interval  $0.8 \text{ MeV} \lesssim \hbar\omega \lesssim 1.2 \text{ MeV}$ ) exceeds that of undulator radiation. This is even more true for high energy electrons (see e.g. figure 4 of [23]). Moreover, the channeling photons are harder than the undulator ones and, therefore, they cannot be easily screened out. This may cause serious problems for many potential applications.

<sup>2</sup>It was argued in [19] that condition (4) is necessary to ensure separation of the undulator radiation and the channeling radiation in the spectrum. In fact, it is not so. The separation is ensured by (3). The latter inequality does follow from (4) when it is supplemented by (5), but (3) can be fulfilled even if  $a_u \lesssim d$ . However, the intensity of the undulator radiation will be small in this case. This is the reason why (4) is necessary in the case of LALP CU.

<sup>3</sup>The centrifugal parameter can be also expressed in the form  $C = R_c/R_{\min}$ , where  $R_c = E/U'_{\max}$  is the critical radius of the channel [20] (also known as Tsyganov's radius) and  $R_{\min} = \lambda_u^2/(4\pi^2 a_u)$  is the minimal curvature radius of a sinusoid with the period  $\lambda_u$  and the amplitude  $a_u$ .

<sup>4</sup>Dechanneling is defined in [21] as crossing the channel boundary. Other authors (see e.g. [22]) define dechanneling as rising the energy of the channeling oscillations above the interchannel barrier. The value of the dechanneling length depends only slightly on the definition that is used for its computation. The difference does not exceed a few hundreds of nanometers.

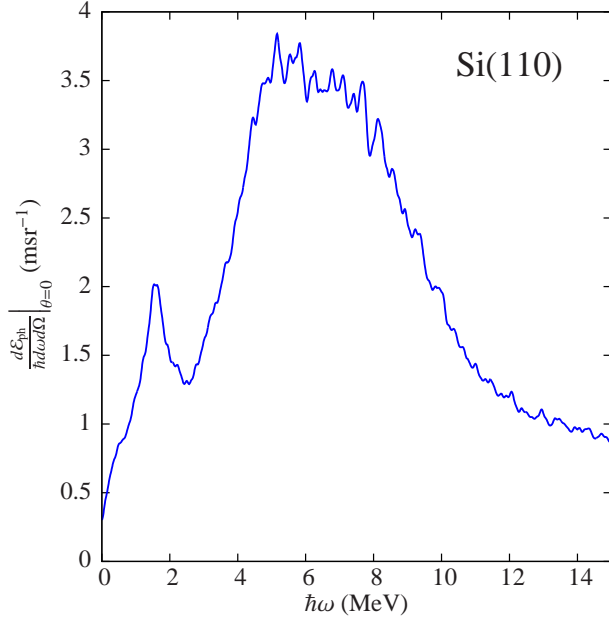


Figure 1: Simulated spectrum of the radiation emitted by  $E = 855$  MeV electrons channeling in a  $24 \mu\text{m}$  long LALPCU with the bending period  $\lambda_u = 4 \mu\text{m}$  and the centrifugal parameter  $C = 0.3$ . The undulator radiation peak is seen at  $\hbar\omega \approx 1.6$  MeV. The spectrum is dominated by channeling radiation (the broad maximum at  $5 \text{ MeV} \lesssim \hbar\omega \lesssim 9 \text{ MeV}$ ).

The results of Monte Carlo simulations shown in figures 1 and 2 were obtained with a new computer code ChaS (**Channeling Simulator**). The code performs a 3D simulation of particle motion in the crystal and calculates the spectral and angular distribution of the emitted radiation.

The previously existing channeling codes can be divided into two main categories. There are codes based on the continuous potential approximation [24, 25, 26, 27, 28, 29, 30] and those considering binary collisions of the projectile with the crystal atoms [31, 32, 33, 34, 35]. In the latter case, the atom is usually taken as a whole, i.e. incoherent collisions with atomic electrons are ignored. In contrast, the algorithm of ChaS is based on the binary collisions of the projectile with target electrons and target nuclei. This novel approach is especially beneficial in the case of negatively charged projectiles, that have to cross the crystal plane during the channeling process. Indeed, the continuous potential approximation becomes inaccurate in the vicinity of the atomic nuclei while the electron density near the crystal plane is much higher than the average one.

The previous version of the code used the electron distribution calculated from Molière's parametrization of the atomic potential. The obtained results were published in [21, 36]. They demonstrated reasonable agreement with experimental data [21]. The present version of ChaS employs a more efficient and robust algorithm for the calculation of the emitted radiation. In addition, it has an option of using the first principle distribution of electrons in the crystal instead of Molière's parametrization. The first principle distribution is calculated within the density functional theory using the computer code ABINIT [37].

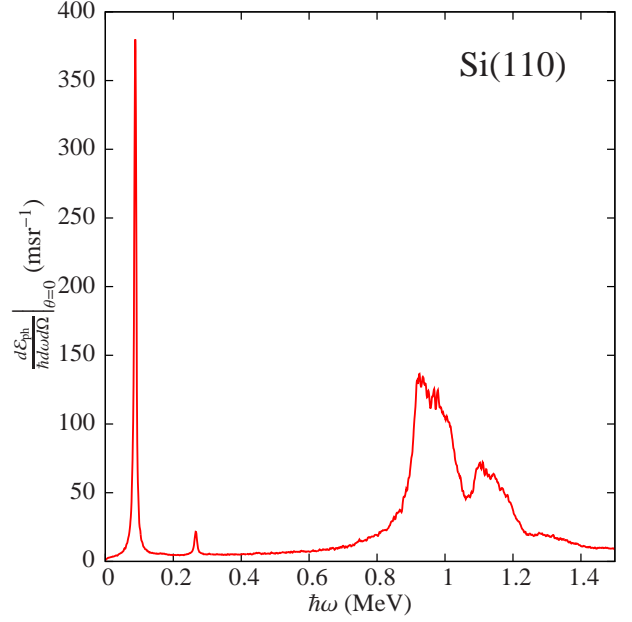


Figure 2: Simulated spectrum of the radiation emitted by  $E = 500$  MeV positrons channeling in a  $350 \mu\text{m}$  long LALPCU with the bending period  $\lambda_u = 23.3 \mu\text{m}$  and the centrifugal parameter  $C \approx 0.12$  ( $a_u = 19.2 \text{ \AA}$ ,  $a_u/d \approx 10$ ). The undulator radiation peak is seen at  $\hbar\omega \approx 88$  keV. The parameters of the crystalline undulator are the same as in right bottom panel of figure 8 of [19]. In contrast to [19], the present simulations take into account the incoherent background.

The code ChaS in its present version is most suitable for the analysis of the channeling of electrons and positrons with energy  $E$  in the range from a few hundreds of MeV to a few GeV with the emission of not very soft:  $\hbar\omega \gtrsim 0.5$  MeV and at the same time not too hard  $\hbar\omega \ll E$  photons. The algorithm takes into account all the physics that is relevant to this domain. A number of phenomena are neglected in the model (e.g. influence of the crystal medium on the emission and propagation of the radiation, quantum effects in the motion of the projectile, losses of the projectile energy due to emission of photons, a shift of the photon energy due to recoil etc.) They are expected to be small and do not influence the results substantially [21, 38].

For simplicity, the emittance of the particle beam was neglected in all simulations presented in this article. The particles were assumed to enter the crystal at zero angle to the crystallographic planes. This is a reasonable approximation in the case of channeling experiments with high quality electron beams [39]. It may not be the case for positron beams, but the beam divergence depends on details of the experimental conditions whose analysis is out of the scope of the present contribution.

It was suggested recently [40] that conditions (4) and (5) are not necessary. In fact, an intense source of hard photons with a narrow spectral distribution can be created if both conditions are violated.

First, let us reanalyze the reasons behind condition (4). It is needed to make sure that the spectrum is dominated by the undulator radiation rather than by the channeling one. However,

the amplitude of undulator oscillations has to be much larger than that of the channeling oscillations only if the frequency of the undulator radiation  $\omega_u$  is smaller than the frequency of channeling oscillations  $\omega_c$ . Indeed, the energy radiated in a certain direction (the forward direction in the present case) by a moving particle in the dipole approximation has the following dependence on the transverse oscillation amplitude  $a$  and the radiation frequency  $\omega$ :

$$\left. \frac{d\mathcal{E}}{d\omega d\Omega} \right|_{\theta=0} \sim a^2 \omega^4. \quad (6)$$

Here  $d\Omega$  is the differential of the solid angle and  $\theta$  is the angle between the direction of the radiation emission and the average direction of the particle motion.<sup>5</sup> Therefore, condition (4) is not necessary, i.e. the amplitude of the undulator bending can be smaller than the channel width,

$$a_u < d, \quad (7)$$

if the frequency of the undulator radiation is considerably larger than that of the channeling radiation

$$\omega_u \gg \omega_c. \quad (8)$$

To fulfill this condition, the period of the crystal bending  $\lambda_u$  has to be much smaller than the smallest period of channeling oscillations  $\lambda_c$ :

$$\lambda_u \ll \lambda_c. \quad (9)$$

The last inequality violates condition (5). This can be seen from the following consideration. The period of the channeling oscillations can be estimated by

$$\lambda_c \simeq 2\pi \sqrt{\frac{E}{U''(0)}}, \quad (10)$$

where  $U''(0)$  is the second derivative of the transverse potential energy with respect to  $y$  in the point of its minimum  $y = 0$  (the axis  $y$  is perpendicular to the channel boundaries). Taking into account that<sup>6</sup>

$$U'_{\max} \lesssim U''(0)d \quad (11)$$

in combination with (10) and (9) one obtains from (5)

$$1 > C \gg \frac{a_u}{d}. \quad (12)$$

The bending amplitude of the crystalline undulator  $a_u$  cannot be much smaller than the channel width  $d$  otherwise it becomes comparable to (or even smaller than) the amplitude of thermal vibrations of the atoms in the crystal. Clearly, the undulator

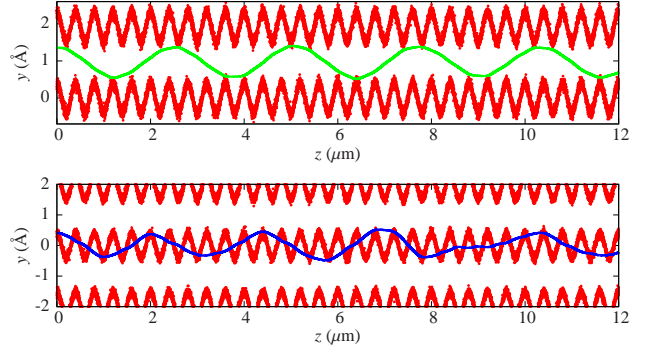


Figure 3: Simulated trajectories of a positron (upper panel) and an electron (lower panel) with energy  $E = 855$  MeV channeling in a crystalline undulator with a small amplitude,  $a_u = 0.4$  Å, and a short period,  $\lambda_u = 400$  nm. The projectile does not follow the shape of the bent crystallographic planes (the thick wavy lines). It performs channeling oscillations with roughly the same period as in a straight crystal. The effect of crystal bending on the shape of trajectories is barely seen. The figure is a modified version of Fig. 1 published in [40].

effect will not be present in this case. If  $a_u$  is comparable to  $d$ , the two inequalities of (12) become incompatible. One might expect that it destroys the undulator effect, but, fortunately, it does not. Condition (5) is, in fact, not applicable in the case of SASP CU (small amplitude (7) and short period (9) crystalline undulator).

In figure 3, simulated trajectories of a positron and an electron channeling in a SASP CU are plotted. One sees from the figure that the particles do not follow the shape of the bent crystallographic planes. Therefore, formula (5) is irrelevant. The channeling process is still present. The particle motion can be roughly considered as if it were governed by a continuous potential averaged over the oscillations of the plane. In other words, it is similar to the channeling in a straight crystal but the average transverse potential is somewhat different.

Still, a more thorough consideration reveals that the particle performs also transverse oscillations with the undulator period  $\lambda_u$ . The amplitude of these oscillations  $a$  is much smaller than the bending amplitude  $a_u$ . Therefore, it is difficult to see the modification of the trajectories induced by the crystal bending in figure 3. Nonetheless, the corresponding Fourier harmonics are present and they are seen in the spectra of the emitted radiation shown in figures 4 and 5.

The undulator radiation peak is higher than the channeling radiation maximum despite of the amplitude  $a$  of the undulator oscillations of the projectile being much smaller than the amplitude of its channeling oscillations  $a_c$ . This seemingly paradoxical fact can be easily understood if relations (6) and (8) are taken into consideration.

The undulator peaks are narrow and well separated from the channeling radiation. The undulator and channeling radiation peaks have approximately the same *absolute* width. Nonetheless, the *relative* width of undulator peaks is much smaller due to (8).

Due to small  $\lambda_u$ , condition (1) can be satisfied for SASP CU even if it is used with a moderate energy electron beam. This

<sup>5</sup>The dependence (6) becomes obvious from the proportionality of the radiated energy to the particle acceleration squared. For transverse harmonic oscillations, the transverse acceleration is proportional to the oscillation frequency squared and linearly proportional to the oscillation amplitude. Hence the dependence (6) is obtained.

<sup>6</sup>Expressions (10) and (11) would be exact equalities in the case of parabolic potential. For a real potential, the second derivative is not constant and the maximum value of the force is reached at  $|y| < d$ , hence (10) is an approximate equality and (11) is an inequality.

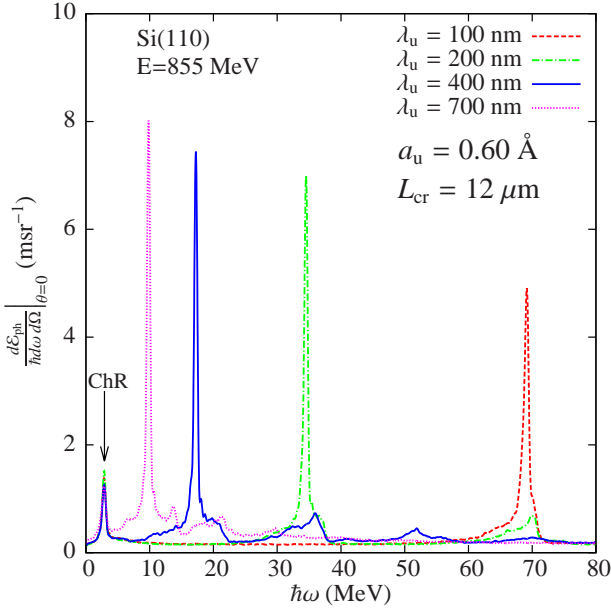


Figure 4: Simulated spectra of the radiation emitted by  $E = 855$  MeV positrons channeling in a  $12 \mu\text{m}$  long crystalline undulator with a small bending amplitude for four short periods. The spectra are obtained by averaging over about 1000 simulated trajectories. The undulator radiation peaks are higher and are centered at a much larger photon energy than the corresponding channeling radiation (ChR) peaks.

is a big practical advantage since electron beams are usually of higher quality and are less expensive than positron ones. Still, positrons are more preferable. As one sees from figures 4 and 5, they allow for a higher intensity of the undulator peak accompanied by a lower background.

The undulator radiation of SASP CU is much harder than the channeling radiation (8). It is an important advantage of SASP CU over LALP CU. It is usually much easier to get rid of a soft photon background and preserve the hard part of the spectrum than to do the opposite. For example, a detector can be made sensitive to hard photons, but be screened from (or made insensitive to) soft photons. It is difficult and sometimes even impossible to do vice versa. For this reason, SASP CU is expected to be much more suitable for many potential applications than LALP CU.

Due to its much smaller bending period, SASP CU can produce by about two orders of magnitude harder photons when used with a beam of the same energy as LALP CU. Or, in other words, SASP CU will require a much smaller and, therefore, a much less expensive accelerator than the one which would be needed for the production of radiation of the same frequency with LALP CU.

Hence, the crystalline undulator that violates conditions (4) and (5) has a number of advantages with respect to LALP CU.

From the technological point of view, SASP CU is more challenging than LALP CU. There exist at least four technologies suitable for the fabrication of LALP CU. The oldest idea of using ultrasonic waves [2, 4] is, unfortunately, still waiting for its experimental implementation. Two other technologies utilize the idea of imposing periodic stresses on the surface of the

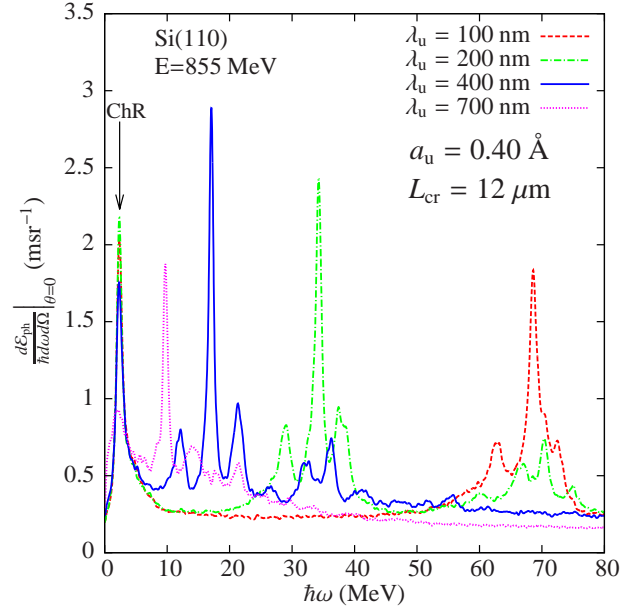


Figure 5: The same as in figure 4 but for electrons. The undulator radiation peaks are lower than in figure 4 by a factor of  $\sim 3$  and the background is higher.

crystal sample. These are making regularly spaced grooves on the crystal surface either by a diamond blade [41, 42] or by means of laser-ablation [43] and deposition of periodic  $\text{Si}_3\text{N}_4$  layers onto the surface of a Si crystal [42]. Finally, there is a way to create periodically varying stresses in the crystal volume by growing a crystal with periodically varying chemical composition. The most mature technology is the creation of strained layer [44] superlattices by periodically varying germanium concentration  $x$  in a  $\text{Si}_{1-x}\text{Ge}_x$  crystal with a periodically varying Ge content  $x$  [45, 46].

The potential applicability of ultrasound in the case of SASP CU requires further investigations. The methods based on surface stresses cannot be applied because they require the transverse dimension of the crystal to be of the order of the bending period [47]. The latter is smaller than  $1 \mu\text{m}$  in the case of SASP CU. Only the last approach, the growing of  $\text{Si}_{1-x}\text{Ge}_x$  strained layer superlattices, is suitable for the fabrication of SASP CU. This technology has been already used for manufacturing the LALP CU that is being used in ongoing experiments at Mainz Microtron [48]. It was demonstrated recently [49] that a  $\text{Si}_{1-x}\text{Ge}_x$  crystalline heterostructure can be grown with the parameters that have been used in the simulations presented in figures 4 and 5. Moreover, the strained layer crystal with parameters of SASP CU was predicted to be stable against misfit dislocations, in contrast to LALP CU which is only metastable.

In conclusion, the crystalline undulator with a small amplitude and a short period can be created and it is predicted to be far superior with respect to LALP CU.

In the present contribution, production of undulator radiation with photon energy in the range of tens of megaelectronvolts is considered. These results are important because the hard photon range is unattainable for the present state-of-the-art

synchrotron radiation sources. It would be, however, interesting to consider production of softer photons, in the range of a few hundreds or even tens of kiloelectronvolts. This domain is on the edge of the capability of the presently existing and constructed facilities [10, 50]. These facilities are, however, unique and very expensive. Due to the fact that SASP CU requires a much smaller accelerator than a conventional undulator for production of photons of the same energy, it has a potential to offer a much less expensive solution. If it were possible to use SASP CU for production of soft X rays, such devices could be made affordable even to medium size university labs or hospitals. A theoretical investigation of the low energy SASP CU is, however, more challenging, because quantum effects definitely cannot be neglected in this case.

Even more exciting future task of this field of science is exploring the possibility to produce coherent radiation with SASP CU [12].

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